



chain nodes :

17 18 25 26 27 28 35 36 37 38 39 40 41 42 43 44 45 46 47 48 49 50 51 52

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 19 20 21 22 23 24 29 30 31 32
33 34

chain bonds :

1-21 2-49 3-18 4-50 8-12 9-51 9-52 10-17 11-45 13-48 14-47 15-44 16-46 18-43
19-26 20-25 21-41 23-28 24-27 28-35 29-37 30-36 31-35 31-42 33-39 34-38 39-40

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10 11-12 11-16 12-13 13-14 14-15
15-16 19-20 19-24 20-21 21-22 22-23 23-24 29-30 29-34 30-31 31-32 32-33 33-34

exact/norm bonds :

3-18 5-7 6-10 7-8 8-9 9-10 10-17 15-44 19-20 19-24 19-26 20-21 20-25 21-22 22-23
23-24 24-27 29-30 29-34 29-37 30-31 30-36 31-32 31-35 32-33 33-34 34-38

exact bonds :

1-21 2-49 4-50 8-12 9-51 9-52 11-45 13-48 14-47 16-46 18-43 21-41 23-28 28-35
31-42 33-39 39-40

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 11-12 11-16 12-13 13-14 14-15 15-16

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:CLASS 18:CLASS 19:Atom 20:Atom 21:Atom
22:Atom 23:Atom 24:Atom 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:Atom 30:Atom 31:Atom
32:Atom 33:Atom 34:Atom 35:CLASS 36:CLASS 37:CLASS 38:CLASS 39:CLASS 40:CLASS 41:CLASS
42:CLASS 43:CLASS 44:CLASS 45:CLASS 46:CLASS 47:CLASS 48:CLASS 49:CLASS 50:CLASS
51:CLASS 52:CLASS